This document is the accepted manuscript version of the following article:
Wu, W., Cronjé, P., Nicolai, B., Verboven, P., Opara, U. L., & Defraeye, T. (2018). Virtual cold chain method to model the postharvest temperature history and quality evolution of fresh fruit – A case study for citrus fruit packed in a single carton. Computers and Electronics in Agriculture, 144, 199-208. http://doi.org/10.1016/j.compag.2017.11.034

Virtual cold chain to model the postharvest thermal history and quality evolution of fresh fruit

– A case study for citrus fruit packed in a single carton

Wentao Wu[1,2], Paul Cronjé[3], Bart Nicolai[4, 5], Pieter Verboven [5], Umezuruike Linus Opara[6, 7], Thijs Defraeye [1, 2*]

[1] *Chair of Building Physics, ETH Zurich, Stefano-Franscini-Platz 5, 8093 Zürich, Switzerland*

[2] *Multiscale Studies in Building Physics, Empa, Überlandstrasse 129, 8600 Dübendorf, Switzerland*

[3] *Citrus Research International, Department of Horticultural Sciences, Stellenbosch University, Stellenbosch 7602, South Africa*

[4] *VCBT, Flanders Centre of Postharvest Technology, Willem de Croylaan 42, 3001 Heverlee, Belgium*

[5] *MeBioS, Department of Biosystems, KU Leuven, Willem de Croylaan 42, 3001 Heverlee, Belgium*

[6] *South African Research Chair in Postharvest Technology, Department of Horticultural Sciences, Stellenbosch University, Stellenbosch 7602, South Africa*

[7] *South African Research Chair in Postharvest Technology, Department of Food Science, Stellenbosch University, Stellenbosch 7602, South Africa*

Abstract

[*] Corresponding author. Tel. +41 (0)58 765 47 90

Email Address: thijs.defraeye@empa.ch (Thijs Defraeye)

Fruit quality loss is highly dependent on the temperature control throughout the postharvest cold chain. Previous research mainly focused on optimizing the cooling performance of single unit operations of a cold chain. Assessing fruit temperature and quality evolution throughout the entire postharvest cold chain is, however, also critical to determine the end quality and incidence of losses. This study proposes a new modelling method – the virtual cold chain (VCC) to predict the temperature-time history and associated quality loss of packaged fresh fruit, down to each individual fruit, all the way from farm to consumer. The VCC method is based on computational fluid dynamics (CFD) combined with kinetic quality modelling. The feasibility and performance of the VCC method are tested by a case study where different citrus cold chains are compared for a single carton of fruit. The difference in quality loss among individual fruit in the carton could reach 11% for a specific cold chain. Among different cold chains that are evaluated, significant differences in remaining quality are also identified, namely up to 23%. The results confirm that the VCC method has a large potential to virtually track temperature-time histories and to estimate quality loss of individual fruit in the cargo throughout a cold chain. The VCC method is therefore a new tool to optimize cold chain strategies and to improve package design.

Industrial relevance text

Postharvest losses of fruit from harvest until they reach the consumer are as high as 13% in Europe and 38% in Africa. Innovative methods to quantify and reduce quality loss at all stages of cold chains are urgently needed. As the virtual cold chain method has the ability to track temperature-time history and quality evolution of each individual fruit in the cargo, it enables the estimation of postharvest losses throughout the cold chain, and the optimization of unit operation conditions in order to reduce fruit losses. A main advantage of the VCC method is that quality loss can be quantified in detail for each individual fruit.

Highlights

► VCC virtually tracks temperature-time histories of each individual fruit.

► Difference in quality loss between individual fruit in a cold chain was 11%.

► Difference in remaining quality for different cold chains was 23%.

Keywords: Cold chain; Precooling; Refrigerated container; CFD; Orange fruit

1. Introduction

A general and growing concern in the fruit industry is the loss of quality in supply chains. Postharvest losses, from the point of harvest until fruit reaches the consumer, can be as high as 13 to 38% (Gustavsson et al., 2011). To reduce the incidence and magnitude of postharvest losses, it is crucial to rapidly remove the field heat of the produce after harvest and to maintain optimum produce temperature throughout the entire supply chain. The reason is that temperature is the single most important factor affecting fresh produce quality change, deterioration rates and shelf life (Thompson et al., 2008; Qiu and Wang, 2015). The temperature-time history of fruit can be directly related to the produce quality loss (Robertson, 1993) and market value. Therefore, tracking the temperature-time history of fresh fruit is essential to estimate quality evolution throughout the cold chain.

To this end, measuring the pulp temperature of fruit, and not the air temperature, is required. Pulp temperatures are monitored, for example, to decide when to stop the precooling process or to evaluate the state of the cargo during overseas maritime transport in refrigerated containers. The core temperature is a conservative quantity as it is the location in the fruit which is the last to reach the target temperature. However, in these commercial operations, these core temperatures are not that easy to measure for packed fruit throughout the entire cold chain. Temperature sensors, such as point probes, are inserted after fruit have been packed in cartons and stacked on pallets. Hence, core temperature-time history is often monitored at locations that are easy to access, such as the side of the pallet and carton, and only a limited amount of fruit are monitored. However, fruit in different locations of pallets, e.g., fruit in top and bottom cartons, do not cool in the same way (Pelletier et al., 2011; Defraeye et al., 2013a; Defraeye et al., 2015). Therefore, the recorded fruit core temperature-time history, tracked at these selected locations, does not necessarily represent the overall fruit quality evolution of a particular cargo.

An alternative method to obtain fruit temperature data at a much higher spatial resolution in the cargo is to apply numerical modelling by computational fluid dynamics (CFD). CFD has been widely applied in postharvest handling and food processing (Ramachandran et al., 2011; Ambaw et al., 2013a; Smith et al., 2014; Tian and Barigou, 2016). The advantage of CFD simulations is that core temperatures of every single fruit in a carton or in a pallet during cooling can be calculated and recorded, as heat transfer within the products and their heat exchange with the surrounding airflow are explicitly modelled (Delele et al., 2013; Defraeye et al., 2014). Because of the added insight it provides, CFD has been successfully applied to model cooling of fruit in single unit operations in the cold chain, including precooling (Ferrua and Singh, 2009a, b, c & 2011; Defraeye et al., 2013a), refrigerated transport container (Moureh et al., 2009a, b; Defraeye et al., 2015) and cold storage (Chourasia and Goswami, 2007; Delele et al., 2009). The loss of fruit quality is, however, determined by the fruit temperature evolution throughout the entire cold chain, where each unit operation is subject to different temperature and ventilation (air speed) conditions. The FRISBEE tool (Gwanpua et al., 2015) is developed to assess food quality along the European cold chain, in which kinetic models are formulated for different quality parameters (e.g., firmness, color, vitamin C) based on overall product temperature. Nevertheless, to the best knowledge of the authors, CFD-based modelling has not been used to study the temperature-time history of fruit throughout an entire cold chain and to link it to fruit quality evolution.

The objective of this study is, therefore, to develop a virtual cold chain method (VCC) for tracking the temperatures of packed fruit throughout the different unit operations of the entire chain, based on CFD modelling. By transferring the temperature distribution of each individual fruit from one unit operation to the next one, the entire cold chain is simulated. These temperature-time information of each individual fruit is used to predict fruit quality loss throughout the entire postharvest supply chain. The unique insights in the temperature-time history and quality evolution of each individual fruit throughout the entire chain provides new ways to assess different packaging designs and cold chain strategies. As a case study, the performance of this method is evaluated by simulating the cooling behavior of citrus fruit packed in a single carton for different cold chain strategies.

2. Materials and methods

2.1. The Virtual cold chain (VCC) method

The VCC method is illustrated for a typical cold chain for citrus fruit, consisting of three unit operations - precooling, refrigerated transport and cold storage (Fig. 1). In the first step, computational models for each different unit operations are created, which include the detailed geometrical model of the package and individual fruit. Secondly, all unit operations in the cold chain are calculated sequentially, where the temperature condition of each fruit is transferred from one operation, e.g., forced air precooling, to the other, e.g., transport. Then the temperature-time history of each individual fruit is extracted from unit operations throughout the entire cold chain and this information is used in a fruit quality model, which calculates the produce quality evolution.

2.2. Different cold chains

The concept and performance of the VCC approach is illustrated by evaluating cooling and quality evolution of citrus fruit packed in a single carton for five cold chain scenarios (see Table 1). Although a single carton is used for calculation in this study, it is sufficient to show the ability of the VCC method, which can be later extended to more comprehensive computational models (e.g. pallet). During forced air precooling, the carton is ventilated with horizontal airflow (See Fig. 2 (a)) and at high airflow rates, typically 0.5-3 L $kg^{-1}s^{-1}$ (Thompson et al., 2008). During refrigerated transport, the carton is ventilated with vertical airflow (See Fig. 2 (a)). In a refrigerated container, the airflow rate is typically 0.02-0.06 L $kg^{-1}s^{-1}$ (Defraeye et al., 2015). During cold storage, the carton is assumed here to be ventilated with horizontal airflow with low airflow rates, which are typically 0.001-0.002 L $kg^{-1}s^{-1}$ (Thompson et al., 2008). Different combinations of these three types of unit operations are evaluated to mimic different postharvest cold chain strategies used in the citrus fruit industry. The baseline cold chain used in this study consists of precooling (1 d at 3 °C), transport (24 d at -1 °C) and cold storage (14 d at 4 °C). This case simulated partial precooling to remove the majority of fruit field heat and then further heat removal during transport. The second cold chain - ‘cold-disinfestation precooling’ - consists of precooling (3 d at -1 °C), transport (24 d at -1 °C) and cold storage (14 d at 4 °C). These lower temperatures are often required for markets demanding a cold disinfestation protocol to kill insect larvae in fruit. The third cold chain - ‘ambient cooling’ - does not include precooling. Instead, fruit are held in static cold storage for 5 d at 3 °C before shipment, which induces a slow cooling process. Afterwards, the fruit go through refrigerated transport (24 d at -1 °C) and cold storage (14 d at 4 °C) after shipment. In the fourth cold chain, called ‘ambient loading’ (Defraeye et al., 2015), the fruit are directly loaded to the refrigerated container after being packed. After 24 d of transport at -1 °C, fruit are held in cold storage for 14 d at 4 °C. Such ambient loading is used in the South African citrus industry to shorten the cold chain and to avoid the use of precooling facilities as there are several regions where they are not present or where there is insufficient precooling capacity. The last cold chain scenario - ‘holding time after precooling’ includes four unit operations: precooling (1 d at 3 °C), cold storage before shipment (5 d at 3 °C), transport (24 d at -1 °C) and cold storage (14 d at 4 °C) after shipment. This cold chain simulates the case where fruit are kept for a few days after precooling at storage set point temperature (3 °C) before being loaded into the container.

2.3. Computational model

A telescopic corrugated fibreboard carton is used (0.4 m ×0.3 m ×0.27 m, see Fig. 2a). The carton has two circular vents on each lateral side, at half height. During precooling and storage, these side vents enable horizontal airflow. The carton has four circular vents and a rectangular slot on top and bottom, respectively, which enable vertical airflow during transport. The carton is filled with 64 orange fruit according to a predetermined staggered pattern and fruit are discretely modelled as spheres with a diameter of 75 mm. To avoid the generation of highly skewed cells near the contact point of two fruit, a gap of about 3 mm is left between the fruits.

Three separate computational models are constructed for precooling, transport and storage (Fig. 2b). In the models for precooling and storage, the carton is ventilated horizontally (Fig. 2a & b), while in the model for transport, the carton is ventilated vertically (Fig.2a & b). The upstream and downstream sections are extended long enough to reduce the impact of inlet and outlet boundary conditions on the flow near the proximity of the box.

At the outlet, a volumetric flow rate is imposed and the value is determined by the specific cold chain unit operation. The flow rates (see Table 1) in the present study are 1 L $kg^{-1}s^{-1}$, 0.02 L $kg^{-1}s^{-1}$ and 0.002 L $kg^{-1}s^{-1}$ for precooling, transport and storage, respectively. At the inlet, the atmospheric pressure is imposed with a low turbulence intensity of 0.1%. The inlet air temperature, or the so-called set-point temperature for the cold chain unit operation, varies with the different cold chain scenarios that are evaluated, as depicted in Fig. 3. The lateral surfaces parallel to the flow direction are treated as symmetry boundary conditions. The cardboard surfaces perpendicular to the flow direction and the fruit surfaces are modelled as no-slip walls with zero roughness. The initial temperature of the fruit and cardboard is taken equal to 21 ºC in this study.

All CFD models are meshed using tetrahedral cells. The mesh for precooling and storage consists of 1.16×10^6 cells and that for transport (vertical airflow) has 1.35×10^6 cells. The spatial discretisation error is estimated by means of Richardson extrapolation (Roache, 1994), which is about 2.5% for the mass flow rate through the carton and 5% for the convective heat transfer coefficient from the citrus fruit.

2.4. Numerical methods

The simulations are performed with the open source CFD code OpenFOAM 2.4.0. Reynolds-averaged Navier-Stokes (RANS) equations with the shear stress (SST) k-ω turbulence model (Menter, 1994) are used to model turbulent flow. Defraeye et al. (2013b) evaluated a series of RANS turbulence models for the flow over a single sphere and found that the SST k-ω model with low-Reynolds number modelling (LRNM) performed exceptionally well. When modelling packages filled with a large number of fruit, such detailed LRNM of the boundary layer is very challenging as it poses difficulties in grid generation and requires large computational resources. Therefore, the wall function approach is often the only feasible option to model the flow in the boundary layer near the no-slip surfaces (e.g., fruit) for large ensembles of fruit. In a previous study (Defraeye et al., 2013a), the RANS SST k-ω turbulence model, in combination with wall functions, was evaluated for cooling of orange fruit using the same package type, similar fruit size and stacking pattern. The good agreement with experimental data indicated that the use of the RANS SST k-ω turbulence model with wall functions was sufficiently accurate. Other studies (Ambaw et al., 2013b; Delele et al., 2009) also confirmed the good performance of the combination of turbulence model and boundary-layer modelling.

The temperature difference between adjacent citrus fruit is small during cooling. Therefore, radiation exchange between fruit inside the stack is considered small compared to convection heat transfer (Defraeye et al., 2013a) and hence, radiation is not modelled. Buoyancy is not taken into account. Heat of respiration is about 50 W/ton for citrus fruit (ASHRAE, 1994) and mass loss from citrus fruit is smaller than 1% after 3 d at -0.5 ºC (Defraeye et al., 2013a). Heat of respiration and latent heat of evaporation due to mass loss are therefore unlikely to have a significant impact on the cooling rate of citrus fruit (Defraeye et al., 2013a) and are not included in the model. The following thermal properties of citrus fruit are used in the simulations: density of 960 kg m^{-3}, thermal conductivity of 0.386 w $m^{-1}K^{-1}$ and specific heat capacity of 3850 J $kg^{-1}K^{-1}$.

The second-order upwind scheme is used to discretize the advection terms of the governing equations. The first time derivative item is discretized by the first-order, bounded, implicit scheme Euler. The SIMPLE algorithm and merged PISO-SIMPLE (PIMPLE) algorithm are used for steady state and transient simulations, respectively.

A special procedure is applied to simulate the cooling process in order to save computational time. Before simulating the transient cooling process, first, a steady flow field calculation is performed for each unit operation. Since no buoyancy is considered in the model, the flow field remains steady over time and does not need to be resolved anymore during the transient simulations. Therefore, only heat transfer is solved during the transient calculations. The transient simulations are run with a time step of 60 s, which is determined from the temporal sensitivity analysis.

2.5. Fruit quality model

The quality loss of perishable fruit over time depends on the temperature conditions from the point of harvest until consumption (Hertog et al., 2014). In this study, the change in overall quality, indicated by parameter A, is estimated based on the simulated fruit temperature (volume-averaged or core) throughout each virtual cold chain. A generic model for the change in quality over time is built up, based on a kinetic rate law (Robertson, 1993):

$$-\frac{dA}{dt} = kA^n \tag{1}$$

where t is the time [s], k is the rate constant [s^{-1}], n is the order of the reaction which determines whether the change of A over time is dependent on itself. A zero-order reaction is assumed in this study for the change of the overall quality A. This implies that the change of A over time is a linear curve, where the magnitude of the slope equals k. Thereby, Eq.(1) can be integrated, resulting in a linear decrease of the quality parameter in case k is a constant at constant temperature:

$$A = A_0 - kt \tag{2}$$

where A_0 is the quality at the start of a cold chain (t = 0 d). The temperature dependency of the degradation of fruit quality is accounted for by the rate constant k, which is often described by an Arrhenius relationship (Robertson, 1993):

$$k(T) = k_0 e^{\frac{-E_a}{RT}} \tag{3}$$

where k_0 is a constant [d^{-1}], E_a is the activation energy [$J\ mol^{-1}$], R is the ideal gas constant (8.314 $J\ mol^{-1}\ K^{-1}$), T is the absolute temperature [K]. To calculate $k(T)$, k_0 and E_a need to be known. They can be inferred from quality decay data.

First, k needs to be known at a certain temperature. According to Cantwell (2001), citrus fruit can be stored for approximately 8 weeks (56 d) at 4 ºC. Therefore, the initial overall quality A_0 is assumed to be 100% at 4 ºC in the beginning (t_0 (4 ºC) = 0 d) and the remaining quality A_{end} at 4 ºC after 8 weeks (t_{end} (4 ºC) = 56 d) equals 0%. This means that 100% of the quality parameter is assumed to be lost after the citrus fruit are stored for 8 weeks at 4 ºC. Based on these quantities, a rate constant at 4 ºC can be derived from Eq. (2), which is 1.79% d^{-1}.

Second, information on the temperature dependency of the rate constant is required. In this study, this information is determined via the Q_{10} value:

$$Q_{10} = \frac{k_{T+10}}{k_T} \tag{4}$$

where k_{T+10} and k_T are the rate constants at temperatures T and T+10 K. The Q_{10} value is typically about 2-3 for degradation reactions in fruit (Robertson, 1993). In this study, a value of 2 is chosen for Q_{10}, which means that an increase in temperature of 10 °C doubles the rate constant. From Eq. (3) and (4), the following equations can be derived:

$$E_a = \frac{R\ln(Q_{10})}{1/T - 1/(T+10)} \tag{5}$$

Based on Q_{10} of 2 and a temperature of 277.15 K, E_a equals 4.59 x 10^4 J mol^{-1}. Based on k(4°C) = 1.79% d^{-1} and E_a, k_0 is equal to 7.89 x 10^6 d^{-1} calculated from Eq. (3).

As fruit temperature varies along the cold chain, the rate constant will also vary accordingly. Fruit core temperatures are extracted at a time interval of 60 s (6.94 x 10^{-4} d) from the CFD simulations. Eq. (3) is then used to calculate the rate constant for each time interval and the remaining quality at each time step.

2.6. Evaluation of cooling rate

The cooling rate of each fruit is assessed by the core temperature-time profile. From these temperature profiles (T [K]) the fractional unaccomplished temperature change (Y) can be determined (Defraeye et al., 2015)

$$Y = \frac{T - T_a}{T_i - T_a} \quad (6)$$

where T is the core temperature of individual fruit, T_i is the initial fruit temperature and T_a is the set point temperature in the associated cold chain unit operation. From the definition of Y, the seven eighths cooling/heating time ($t_{7/8}$) can be determined, which is the time required to reduce the temperature difference between the fruit and the approaching airflow by seven eights (Y=0.125). A more detailed explanation and use of this parameter can be found in the work of Defraeye et al. (2015).

Besides $t_{7/8}$, the convection heat transfer coefficient (CHTC) is also used to assess the cooling heterogeneity of fruit under different unit operations:

$$CHTC = \frac{q_{cw}}{T_w - T_a} \quad (7)$$

where q_{cw} is the convection heat flux normal to the surface (J s^{-1} m^{-2}), i.e., at the air-fruit interface and T_w (K) is the fruit surface temperature.

3. Results

3.1. Heterogeneity of cooling and quality loss among individual fruit for the baseline cold chain

The advantages of applying the VCC method to assess fruit quality loss is demonstrated by evaluating cooling heterogeneity and variations in quality loss of individual fruit for the baseline cold chain. Fruit cooling behavior is assessed first from the fruit core temperature-time history of each individual fruit in the carton (Fig. 4). The spatial distribution of $t_{7/8}$ for the individual fruit is depicted in Fig. 5. The seven-eighths cooling/heating time ($t_{7/8}$) facilitates quantitative comparison of cooling behavior and heterogeneity, as only a single value is obtained for each individual fruit per cold chain operation. During precooling, the $t_{7/8}$ varies from 0.1 d (about 2.4 h) to 0.2 d (about 4.8 h) for different fruit. The core temperature profiles clearly show a spread, which indicates cooling heterogeneity between the individual fruits. In the precooling process, the two middle layers of fruit along the height of the box, and particularly the centrally located fruit cool faster than the two outer layers. This is due to the fact that the vent holes are located along the position of these fruit. In the refrigerated container, the difference in $t_{7/8}$ is about 2.2 d between the fastest and slowest cooling fruit. The spread of the core temperature profiles is clearly larger than precooling, due to the lower airflow rates. During transport, $t_{7/8}$ is more closely related to the distance from the fruit to vent holes on the flow inlet side, due to the fact that there are more vent holes, leading to more uniform cooling of fruit at a particular distance from the inlet. During storage, the core temperature of individual fruit does not even reach the set point temperature after 14 d due to the low airflow rates. The spread in the temperature profiles is much larger compared to precooling and transport. For storage, a closer dependency on the distance from the fruit to the inlet is found than for precooling, which is caused by the lower air speeds and thus different airflow field inside the carton. The lower the airflow rates lead to the slower cooling rate and the higher cooling heterogeneity. Note that in commercial cold chain operations, much larger quantities of fruit are cooled, e.g. a pallet, which have a larger thermal mass, and thereby will be cooled a bit slower than the fruit in the single carton of the present case study.

Besides the temperature-time profiles and $t_{7/8}$, the CHTC, obtained from the steady simulations of each unit operation, is used as a measure of the cooling heterogeneity between individual fruit. For this purpose, the CHTC at the surfaces of the fruit is calculated for precooling, transport and storage. The CHTC of each computational cell on the surface of each fruit is calculated. The relative frequency distribution of the CHTCs is shown in Fig. 6. These CHTCs are scaled with the average CHTC of all fruit in the carton in the same way as Defraeye et al. (2013a). For the precooling process, with high airflow rates, the CHTC distribution is more uniform. For transport and storage processes, the relative frequency distribution shows a larger spread and becomes more skewed towards smaller CHTCs.

The quality loss of each individual fruit throughout the baseline cold chain is shown in Fig. 7. After 1 d precooling, all fruit have about the same quality loss of 3%. During refrigerated transport, the quality loss starts to vary for different fruit. During storage, the variation of quality loss becomes even larger, due to the temperature differences between the individual fruit. At the end of the cold chain, the difference in remaining quality between individual fruit is 4%. Note that although these differences might seem rather small, they are expected to increase when larger number of fruit are considered, such as an entire pallet or a container. Furthermore, the overall quality loss is considered here, so for other more specific quality parameters, these differences can be also more pronounced, depending on the rate constants.

3.2. *Differences in temperature history and fruit quality loss for five different cold chain scenarios*

The VCC method is used to compare the temperature-time history and the quality loss of fruit throughout the baseline and four alternative cold chains (see Table 1). The volume averaged temperature history of all fruit (Fig. 8) is used to compare the differences of the five cold chains in a concise way. The cold-disinfestation precooling cold chain is the most efficient strategy to lower the fruit temperature. The baseline cold chain and the cold chain - holding time after precooling are also efficient to cool the fruit quickly to 3 °C. Compared to the cold chains with precooling, it takes about 2 d longer to bring the down the fruit temperature to 3 °C in the ambient loading cold chain. The field heat in the fruit cannot be rapidly removed in the ambient cooling cold chain due to very low airflow rates in cold storage before shipment, which makes that the fruit remain at higher temperatures for a longer time.

The core temperature-time history of individual fruit is shown in Fig. 9 for all cold chain scenarios. In the cold-disinfestation precooling cold chain, precooling is able to bring down the temperature to -1 °C within 0.5 d. Fruit temperatures stay around -1 °C during transport. During storage, the fruit temperatures increase due to the higher set point temperature. In the ambient cooling cold chain, fruit temperatures stay between 9.1 °C to 20 °C after 5 d of cooling. The cooling of the fruit is slower due to the lower airflow rates. In the ambient loading cold chain, all fruit temperatures decrease to -1 °C within 5 d. As such this technique has a promising potential to remove the entire field heat of fruit during transport. The temperature profiles are very similar between the cold chain – holding time after precooling and the baseline cold chain. The reason is that the precooling reduces the fruit temperature already sufficiently so the subsequent storage before shipment does not affect the fruit temperature significantly. However, the longer duration of the cold chain - partial precooling plus cold storage (5 more days) will affect fruit quality, as discussed below.

An important aim of the VCC method is to estimate the remaining fruit quality at the end of the cold chain for individual fruit in the cargo. The ensemble quality evolution of all fruits in the five cold chains is presented in Fig. 10. The quality evolution is calculated from the volume-averaged fruit temperature. The remaining quality is 47%, 46%, 24%, 46% and 39% for baseline, cold-disinfestation precooling, ambient cooling, ambient loading and holding time after precooling cold chains, respectively. The higher remaining quality for the baseline cold chain is due to the fast precooling and also shorter total duration of the cold chain. The ambient cooling cold chain has the minimum remaining quality with about 23% higher quality loss compared to the baseline cold chain. The reason is that during cold storage before shipment, fruit temperatures are higher (Fig. 8). During the first five days, there is a large quality loss of 23%, which indicates the importance of precooling after harvest. Compared to the remaining quality of the partial precooling cold chain, the cold chain – holding time after precooling has about 8% more quality loss. This is caused by the 5 d delay before transport, which clearly has a significant impact. Comparing the quality loss within the same amount of days (the ambient cooling cold chain and the cold chain – holding time after precooling), it is clear that precooling first and storage afterwards has a beneficial effect on quality. Ambient loading shows an obvious deviation from the precooling-based cold chains in the beginning. The reason is that the airflow rate (0.02 L $kg^{-1}s^{-1}$) during transport removes the field heat slower.

The quality loss of individual fruit (Fig. 11) is presented for the most efficient (cold-disinfestation precooling) and the most inefficient (ambient cooling) cold chain. Individual fruit have a small difference in quality loss in the cold-disinfestation precooling cold chain with a maximum difference of 3%. However, a large spread of quality loss is found for the fruit in the ambient cooling cold chain, with a maximum difference of 11%.

4. Discussion

4.1. Advantages of the VCC method

The major advantage of the VCC method is that temperature-time history is obtained for each individual fruit throughout the entire cold chain. In the fruit industry, a primary challenge is to improve cooling rate and uniformity during postharvest unit operations, by which a priority is to understand the cooling behavior of individual fruit. By means of the VCC method, such temperature-time history can be quantified in detail for each individual fruit (Fig. 4, Fig. 8 & Fig. 9) throughout the entire chain. In experiments, only the core temperatures of a limited number of fruit are monitored in locations that are easy to access. The VCC method overcomes these disadvantages by virtually tracking the thermal history of each individual fruit.

The second advantage of the current VCC method is that it includes a fruit quality loss model in addition to the calculation of the temperature-time history, to predict the remaining fruit quality (Fig. 7). Many CFD studies (Defraeye et al., 2013a, 2015; Delele et al., 2009; Ferrua and Singh, 2009a, b, c & 2011) have focused on the cooling performance of single unit operations and have not incorporated fruit quality modelling so far. Additional insight is gained by quantifying the percentage quality loss per unit operation of each individual fruit subject to different cold chain scenarios.

4.2. Future applications of VCC method

The VCC method has been demonstrated for a single carton for five different cold chain scenarios. The next step is to apply the VCC method for larger cargo ensembles, such as a pallet. It will offer even more insights on the cooling heterogeneity and variations of individual fruit quality in fruit supply chains, and the authors are currently exploring this. In addition, the VCC method could help to improve package design. By using of the VCC method, the cooling uniformity of newly designed packaging can be evaluated throughout the entire cold chain to evaluate their efficacy. This is an important aspect, as some packages are optimized for forced air precooling (horizontal airflow) but do not cool well under vertical airflow, which would be a problem when ambient loading protocols are used. Another potential of the VCC method is to optimize cold chain strategies. According to the comparison of the partial precooling and the full precooling cold chain, based on fruit temperature history (Fig. 4 & 8) and fruit quality loss (Fig. 7, 10 & 11), it might be an indication that a higher set point temperature and thus a shorter duration of precooling (partial precooling) can keep similar fruit quality. An important future step is to include more elaborate quality kinetics models for separate quality attributes (e.g. vitamin C, (Gwanpua et al., 2015)) and models that do not only depend on temperature, but also on gas conditions for example. In summary, VCC method can help to identify the most efficient cold chain strategy.

5. Conclusion

The virtual cold chain (VCC) method was proposed to virtually track the temperature-time history and quality loss of individual fruit during postharvest handling and transport. The performance of the VCC method was illustrated for a single carton throughout five cold chains. The main conclusions are the following:

- The VCC method was successfully used to virtually track temperature-time history of each individual fruit throughout several different cold chains. The seven-eighths cooling/heating time and the frequency distribution of convection heat transfer coefficient (CHTC) from the VCC method enabled the assessment of the cooling heterogeneity of individual fruit in a carton throughout an entire cold chain. Both parameters showed that higher airflow rates resulted in better cooling uniformity.
- The VCC method enabled also predictions of quality evolution for each individual fruit throughout the cold chain. Within a cold chain, up to 11% differences in end quality between individual fruit in a single carton were found for a certain cold chain. Between the five different cold chains that were evaluated, up to 23% differences in average remaining fruit quality were found.

Acknowledgements

The authors would like to thank the Coop Research Program of the ETH Zurich World Food System Center and the ETH Foundation for supporting this project. U.L. Opara also acknowledges support by the South African Research Chairs Initiative of the Department of Science and Technology and National Research Foundation. We also acknowledge the support of the Swiss National Science Foundation SNSF (project 200021_169372).

References

Ambaw, A., Delele, M.A., Defraeye, T., Ho, Q.T., Opara, U.L., Nicolaï, B.M., Verboven, P., 2013a. The use of CFD to characterize and design post - harvest storage facilities: Past, present and future. Computers and Electronics in Agriculture 93, 184 - 194.

Ambaw A., Verboven P., Delele M.A., Defraeye T., Tijskens E., Shenk A., Nicolai B., 2013b. CFD modelling of the 3D spatial and temporal distribution of 1-methylcyclopropene in a fruit storage container, Food and Bioprocess Technology 6 (9), 2235-2250.

ASHRAE, 1994. ASHRAE Handbook - Refrigeration: systems and applications (SI edition). ASHRAE, Atlanta, USA.

Cantwell, M., 2001. Properties and recommended conditions for long-term storage of fresh fruits and vegetables, UC Davis.

Chourasia, M.K., Goswami, T.K., 2007. Steady state CFD modelling of airflow, heat transfer and moisture loss in a commercial potato cold store. International Journal of Refrigeration 30, 672–689.

Defraeye T., Lambrecht R., Ambaw A., Delele M.A., Opara U.L., Cronjé P., Verboven P., Nicolai B., 2013a. Forced-convective cooling of citrus fruit: package design, Journal of Food Engineering 118 (1), 8-18.

Defraeye T., Verboven P., Nicolai B., 2013b. CFD modelling of flow and scalar exchange of spherical food products: turbulence and boundary layer modelling, Journal of Food Engineering 114 (4), 495-504.

Defraeye T., Lambrecht R., Delele M.A., Ambaw A., Opara U.L., Cronjé P., Verboven P., Nicolai B., 2014. Forced-convective cooling of citrus fruit: cooling conditions and energy consumption in relation to package design, Journal of Food Engineering 121, 118-127

Defraeye T., Verboven P., Opara U.L., Nicolai B., Cronjé P., 2015. Feasibility of ambient loading of citrus fruit into refrigerated containers for cooling during marine transport, Biosystems Engineering 134, 20-30.

Delele, M.A., Schenk, A., Ramon, H., Nicolaï, B.M., Verboven, P., 2009. Evaluation of a chicory root cold store humidification system using computational fluid dynamics. Journal of Food Engineering 94, 110–121.

Delele, M.A., Ngcobo, M.E.K., Getahun, S.T., Chen, L., Mellmann, J., Opara, U.L., 2013. Studying airflow and heat transfer characteristics of a horticultural produce packaging system using a 3‐D CFD model. Part I: Model development and validation. Postharvest Biology and Technology 86, 536–545.

Ferrua, M.J., Singh, R.P., 2009a. Modeling the forced-air cooling process of fresh strawberry packages, Part I: numerical model. International Journal of Refrigeration 32, 335–348.

Ferrua, M.J., Singh, R.P., 2009b. Modeling the forced-air cooling process of fresh strawberry packages, Part II: experimental validation of the flow model. International Journal of Refrigeration 32, 349–358.

Ferrua, M.J., Singh, R.P., 2009c. Modeling the forced-air cooling process of fresh strawberry packages, Part III: experimental validation of the energy model. International Journal of Refrigeration 32, 359–368.

Ferrua, M.J., Singh, R.P., 2011. Improved airflow method and packaging system for forced-air cooling of strawberries. International Journal of Refrigeration 34, 1162–1173.

Gwanpua, S., Verboven, P., Leducq, D., Brown, T., Verlinden, B., Bekele, E., Aregawi, W., Evans, J., Foster, A., Duret, S., Hoang, H., van der Sluis, S., Wissink, E., Hendriksen, L., Taoukis, P., Gogou, E., Stahl, V., El Jabri, M., Le Page, J., Claussen, I., Indergård, E., Nicolai, B., Alvarez, G., Geeraerd, A., 2015. The FRISBEE tool, a software for optimising the trade-off between food quality, energy use, and global warming impact of cold chains.

Journal of Food Engineering 148, 2-12.

Gustavsson, J., Cederberg, C., Sonesson, U., van Otterdijk, R., Meybeck, A., 2011. Global food losses and food wastes – extent, causes and prevention (www.fao.org). Rome, Italy.

Hertog, M.L.A.T.M., Uysal, I., Mccarthy, U., Verlinden, B.M., Nicolaï, B.M., 2014. Shelf life modelling for first - expired - first - out warehouse management. Philosophical Transactions of the Royal Society A 372, 20130306.

Menter, F.R., 1994. Two equation eddy viscosity turbulence models for engineering applications. AIAA Journal 32(8), 1598-1605.

Moureh, J., Tapsoba, S., Derens, E., Flick, D., 2009a. Airflow in a slot-ventilated enclosure partially filled with porous boxes: Part I – measurements and simulations in the clear region. Computers & Fluids 38, 194–205.

Moureh, J., Tapsoba, S., Derens, E., Flick, D., 2009b. Airflow in a slot-ventilated enclosure partially filled with porous boxes: Part II – measurements and simulations within porous boxes. Computers & Fluids 38, 206–220.

Pelletier, W., Brecht, J.K., Nunes, M., Émond J.P., 2011. Quality of Strawberries Shipped by Truck from California to Florida as Influenced by Postharvest Temperature Management Practices. HortTechnology 21(4), 482-493.

Qiu, S., Wang, J., 2015. Effects of storage temperature and time on internal quality of satsuma mandarin (Citrus unshiu marc.) by means of E-nose and E-tongue based on two-way MANOVA analysis and random forest. Innovative Food Science & Emerging Technologies 31, 139-150.

Ramachandran, R., Malhotra, D., Anishaparvin, A., Anandharamakrishnan, C., 2011. Computational fluid dynamics simulation studies on pasteurization of egg in stationary and rotation modes. Innovative Food Science & Emerging Technologies 12 (1), 38-44.

Roache, P., 1994. Perspective: a method for uniform reporting of grid refinement studies. Transactions of the ASME – Journal of Fluids Engineering 116 (3), 405-413.

Robertson, G.L., 1993. Food Packaging: Principles and Practices, Marcel Dekker, Inc., New York.

Smith, N., Knoerzerc, K., Ramosa, A., 2014. Evaluation of the differences of process variables in vertical and horizontal configurations of High Pressure Thermal (HPT) processing systems through numerical modelling. Innovative Food Science & Emerging Technologies 22, 51-62.

Thompson, J. F., Mitchell, F. G., Rumsey, R. T., Kasmire, R. F., & Crisosto, C. H., 2008. Commercial cooling of fruit, vegetables and flowers (p. 61). California: University of California.

Tian, S., Barigou, M., 2016. Using chaotic advection to enhance the continuous heat-hold-cool sterilisation process. Innovative Food Science & Emerging Technologies 34, 352-366.

Fig. 1 The Virtual Cold Chain (VCC) method illustrated for a typical cold chain consisting of precooling, refrigerated transport and cold storage.

Fig. 2 (a) Geometry and dimensions of the package; (b) Computational models and boundary conditions for precooling, transport and storage.

Fig. 3 Flow rate, set point temperature as a function of duration of different cold chains. Green, orange, blue and purple lines symbolize precooling (1 L $kg^{-1}s^{-1}$), storage before shipment (0.002 L $kg^{-1}s^{-1}$), transport (0.02 L $kg^{-1}s^{-1}$) and storage (0.002 L $kg^{-1}s^{-1}$), respectively.

Fig. 4 Core temperature-time history of each individual fruit during each unit operation (precooling, transport and storage) throughout the baseline cold chain.

Fig. 5 Spatial distribution of seven-eighth cooling/heating time ($t_{7/8}$) for each individual fruit during precooling, transport & storage in the baseline cold chain.

Fig.6 Relative frequency distribution of the convection heat transfer coefficient (CHTC) for all fruit during precooling, transport and storage in the baseline cold chain. The CHTCs are scaled with the average CHTC of all fruit.

Fig. 7 Quality loss of each individual fruit throughout the baseline cold chain.

Fig. 8 Volume-averaged temperature-time history of all fruit in the five cold chains.

Fig. 9 Core temperature-time history of each individual fruit during unit operations (precooling, storage before shipment, transport and storage) in the four alternative cold chains.

Fig. 10 Average Quality loss of all fruit in the five cold chains.

Fig. 11 Quality loss of individual fruit in the first and second alternative cold chain.

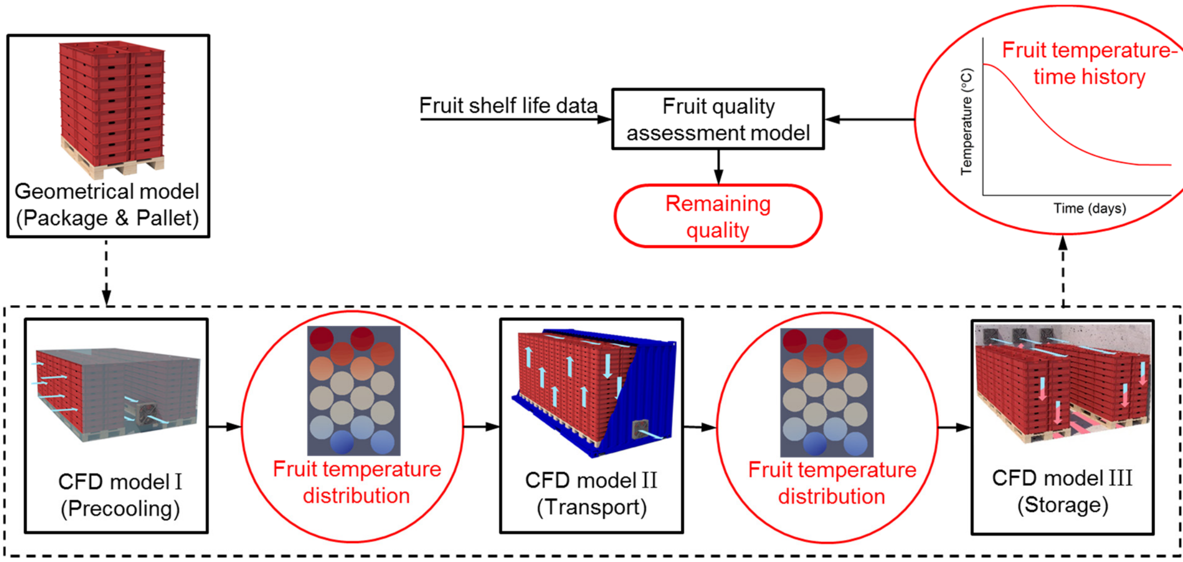

Fig. 1 The Virtual Cold Chain (VCC) method illustrated for a typical cold chain consisting of precooling, refrigerated transport and cold storage.

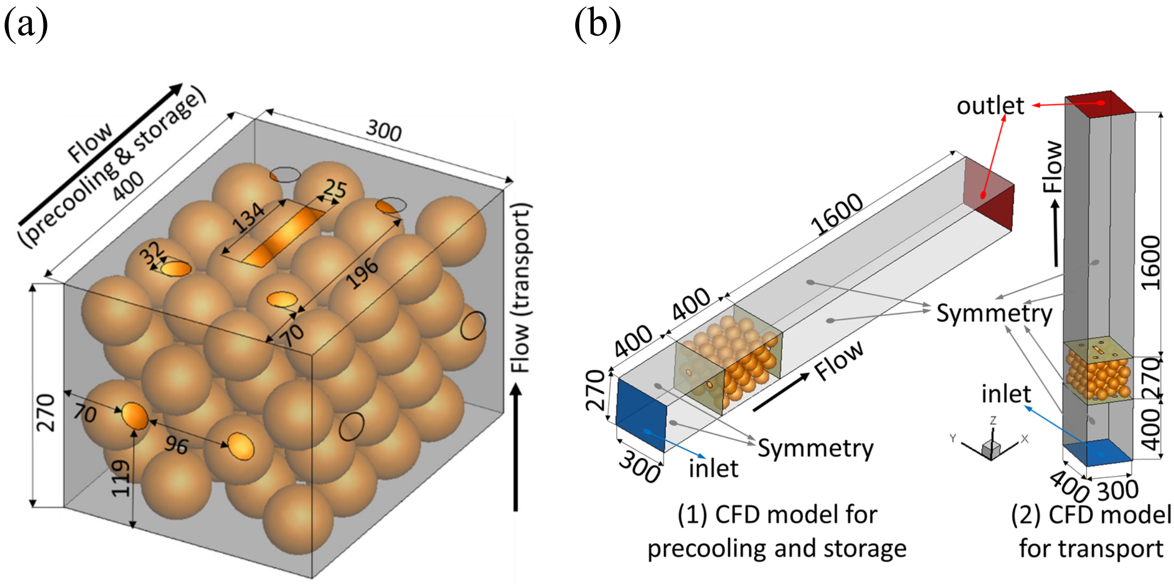

Fig. 2 (a) Geometry and dimensions of the standard package; (b) Cold chain CFD models and boundary conditions for precooling, transport and storage.

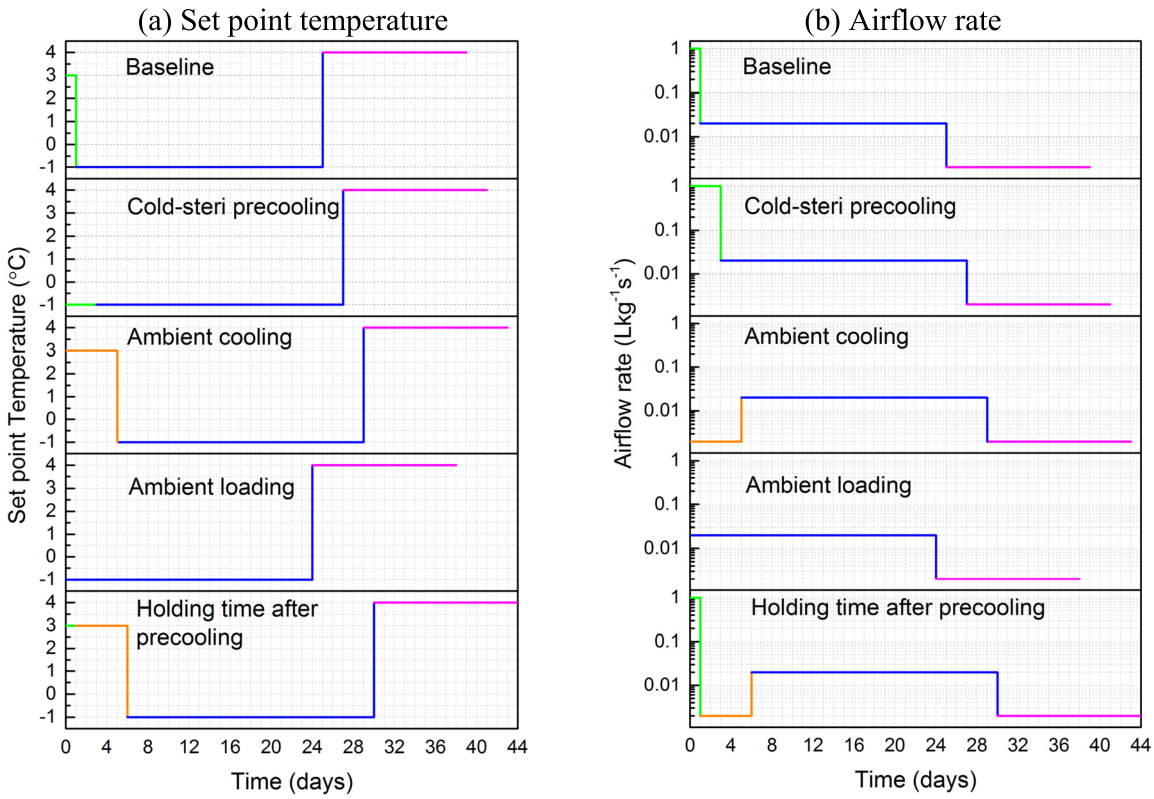

Fig. 3 Flow rate, set point temperature as a function of duration of different cold chains. Green, orange, blue and purple lines symbolize precooling (1 L kg^{-1}s^{-1}), storage before shipment (0.002 L kg^{-1}s^{-1}), transport (0.02 L kg^{-1}s^{-1}) and storage (0.002 L kg^{-1}s^{-1}), respectively.

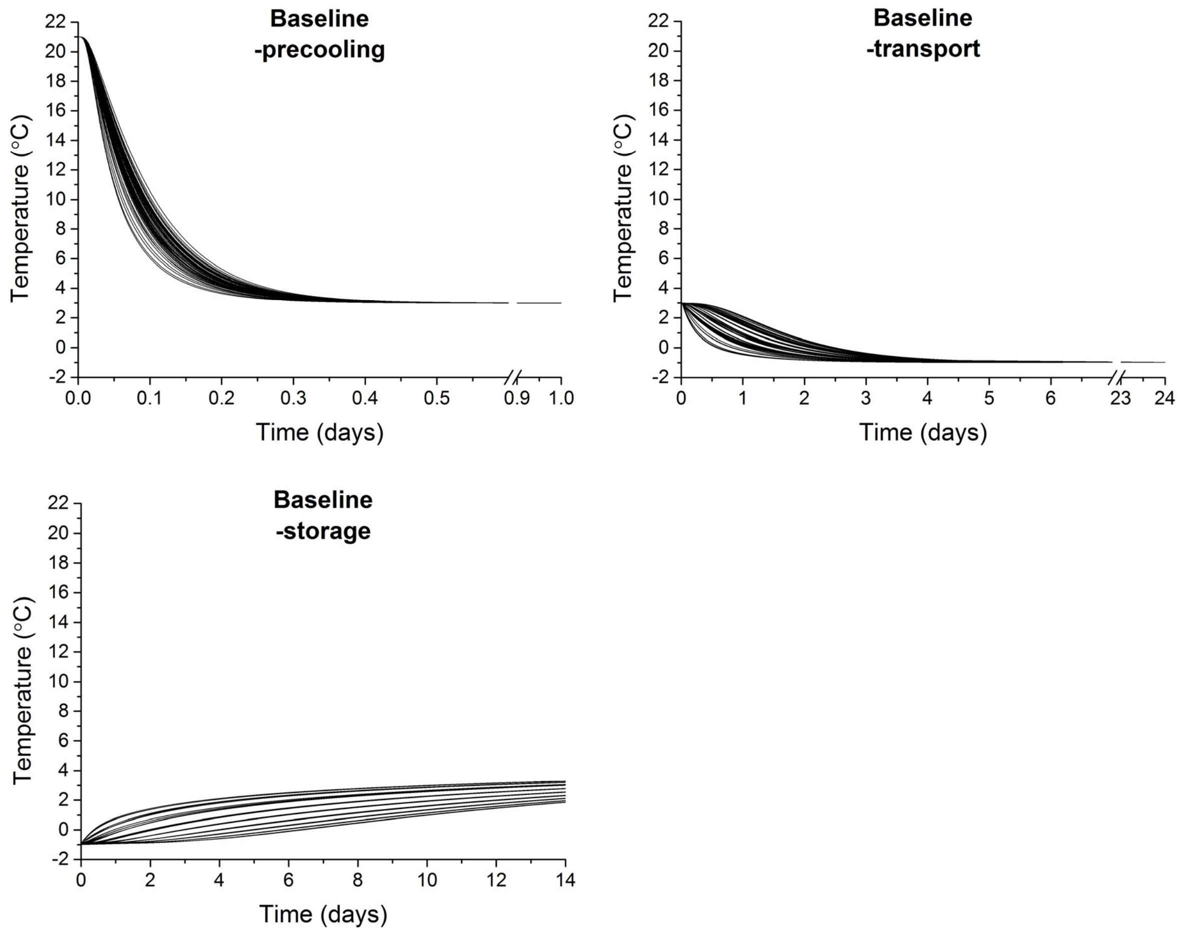

Fig. 4 Core temperature-time history of each individual fruit during each unit operation (precooling, transport and storage) throughout the partial baseline cold chain.

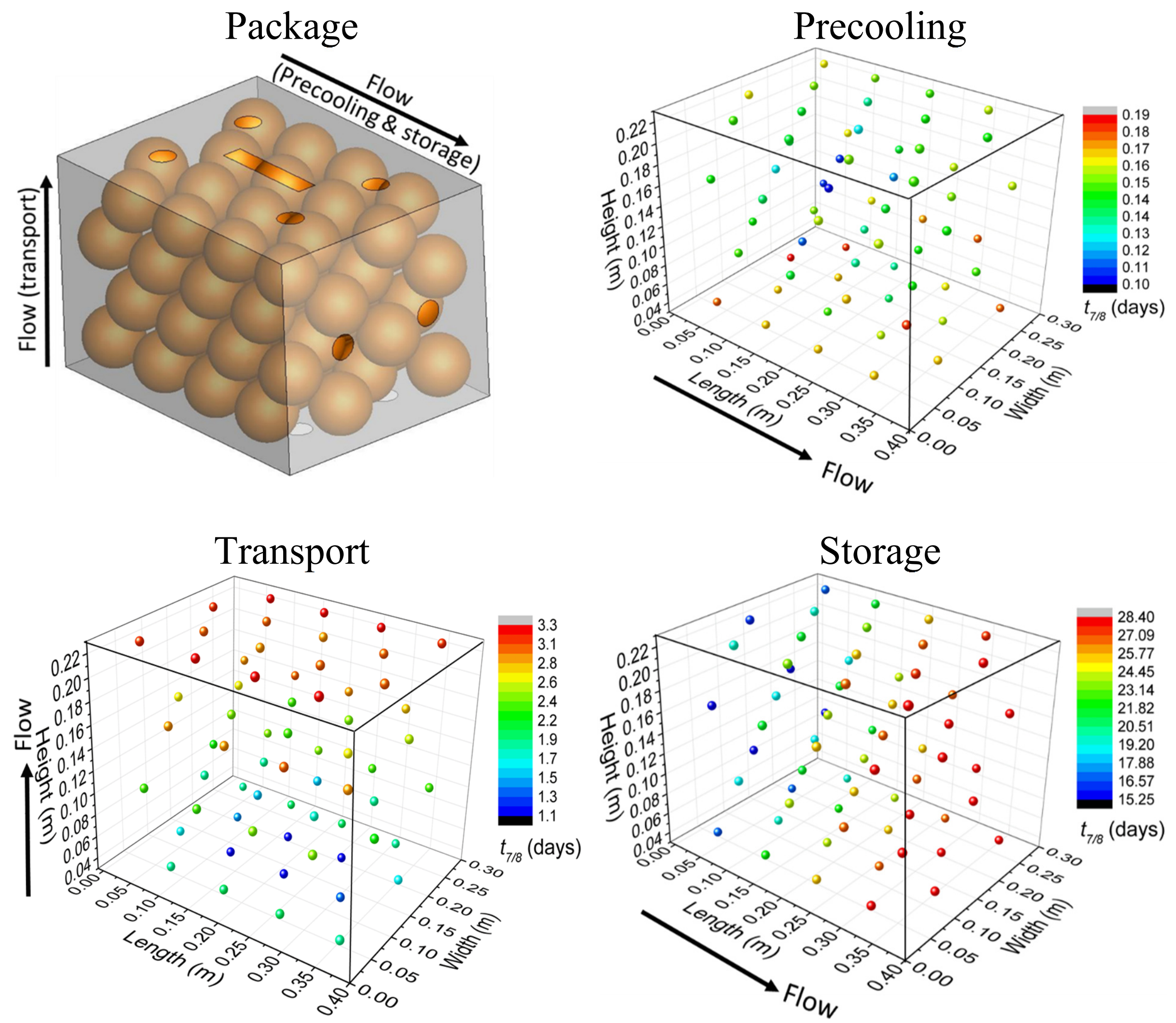

Fig. 5 Spatial distribution of seven-eighth cooling/heating time ($t_{7/8}$) for each individual fruit during precooling, transport & storage in the baseline cold chain.

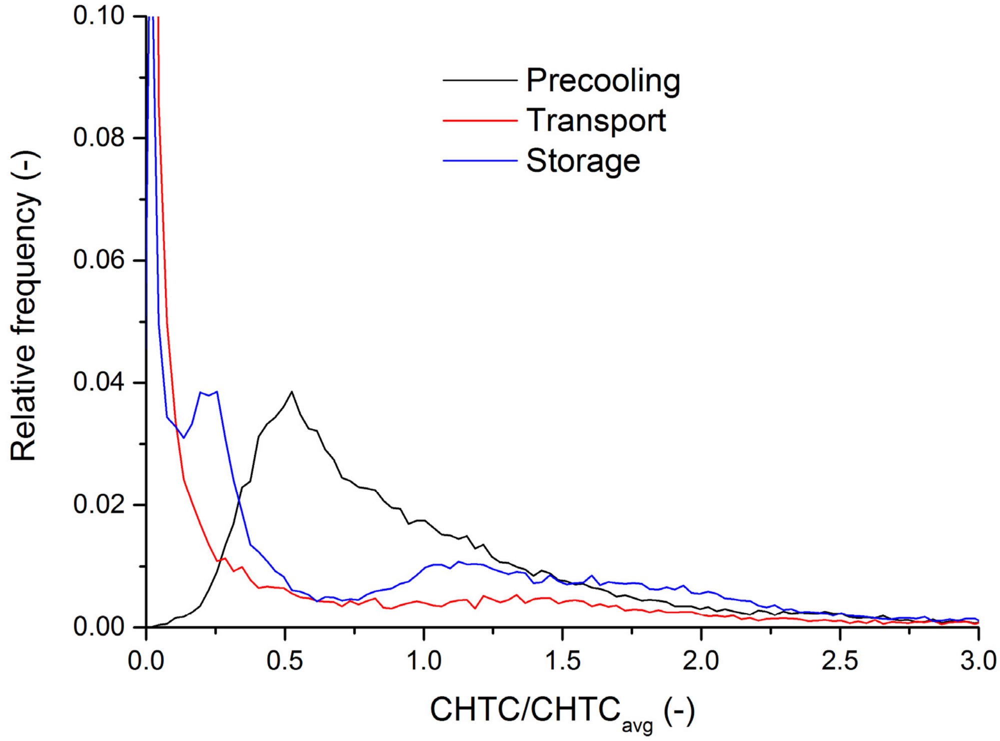

Fig.6 Relative frequency distribution of the convection heat transfer coefficient (CHTC) for all fruit during precooling, transport and storage in the baseline cold chain. The CHTCs are scaled with the average CHTC of all fruit.

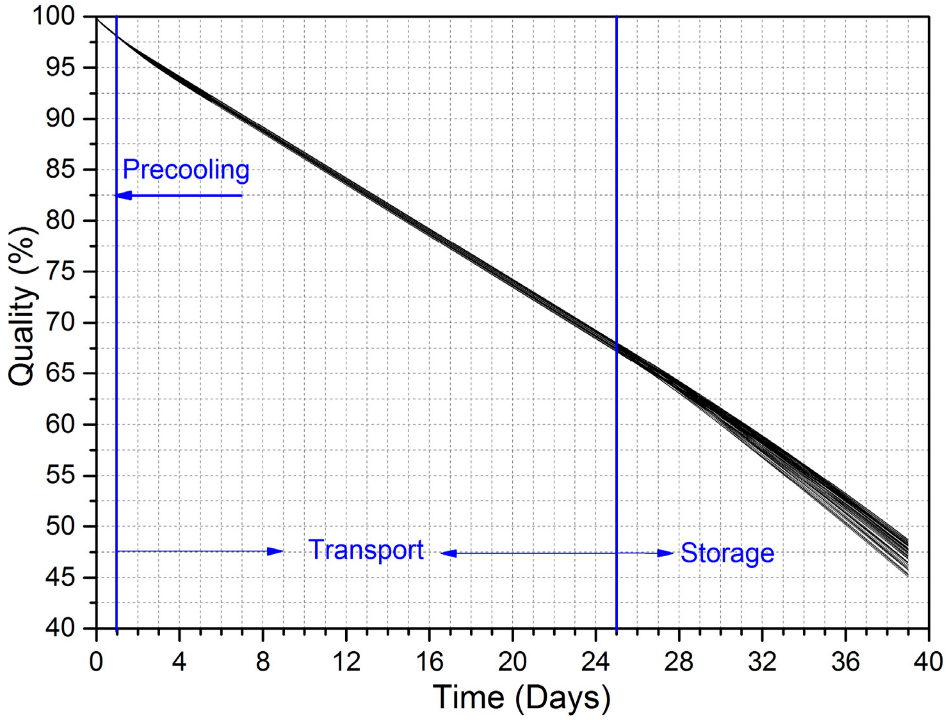

Fig. 7 Quality loss of each individual fruit throughout the baseline cold chain.

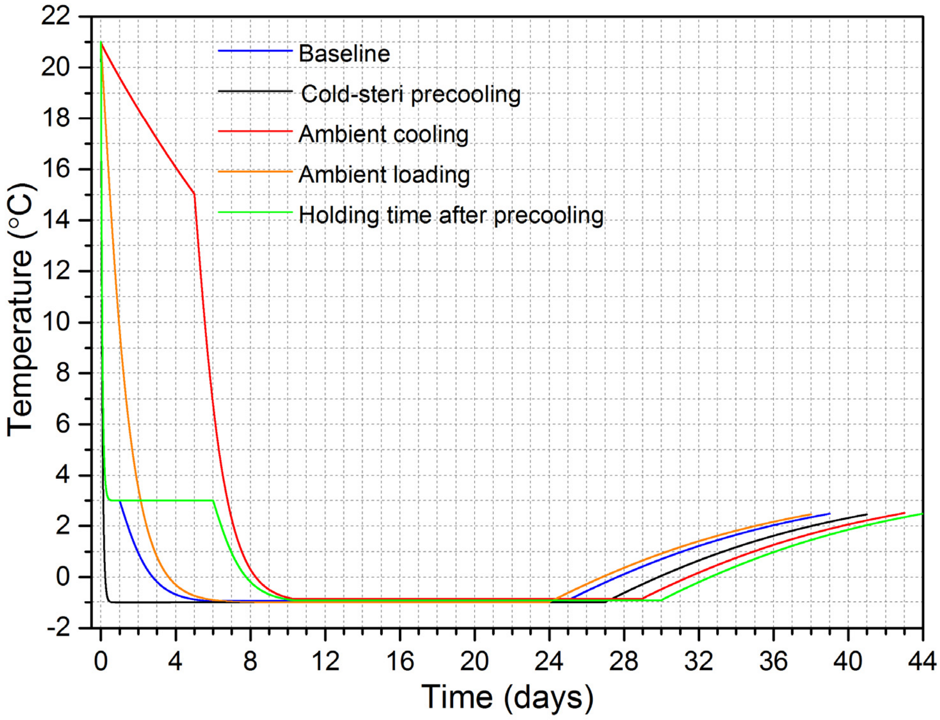

Fig. 8 Volume-averaged temperature-time history of all fruit in the five cold chains.

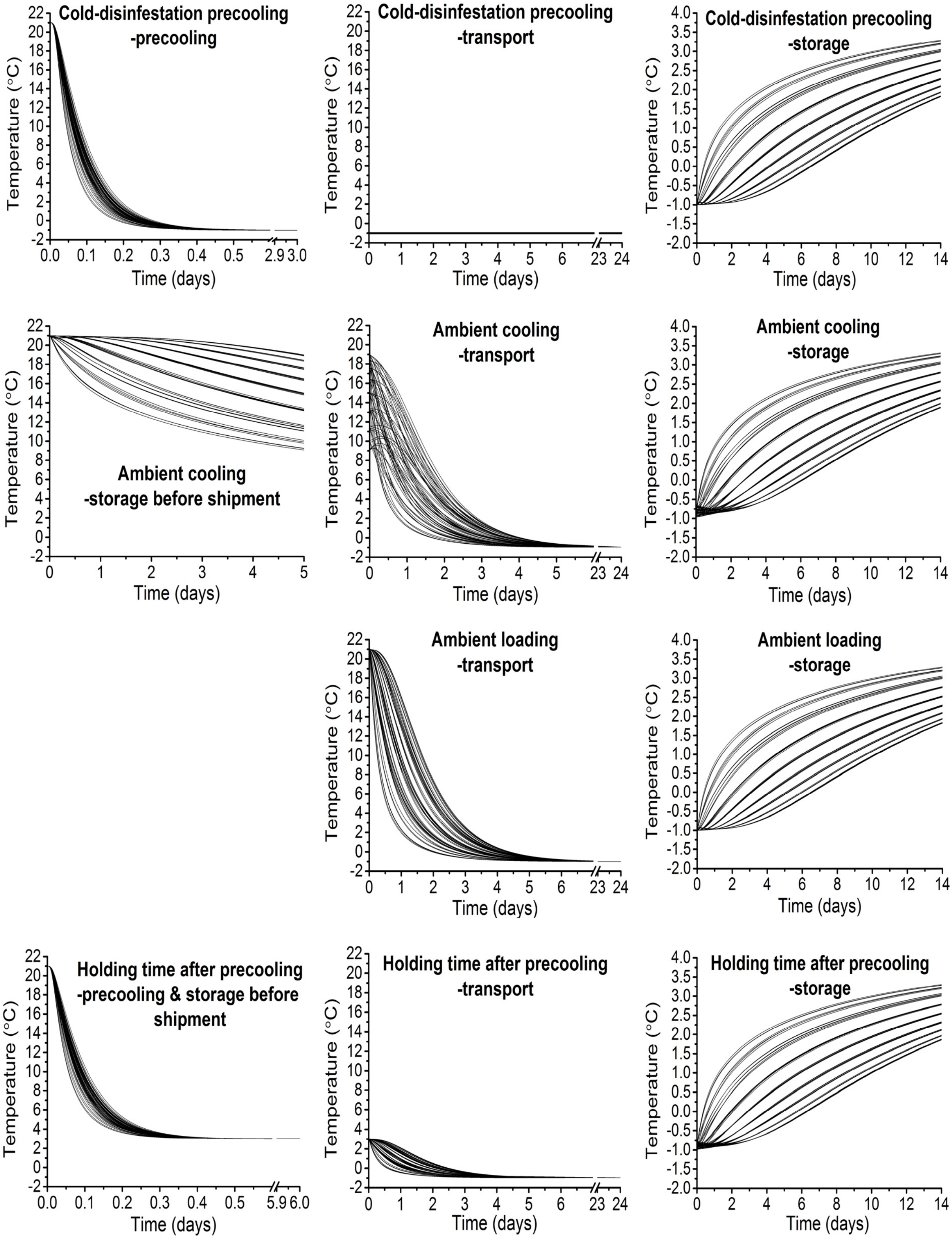

Fig. 9 Core temperature-time history of each individual fruit during unit operations (precooling, storage before shipment, transport and storage) in the four alternative cold chains.

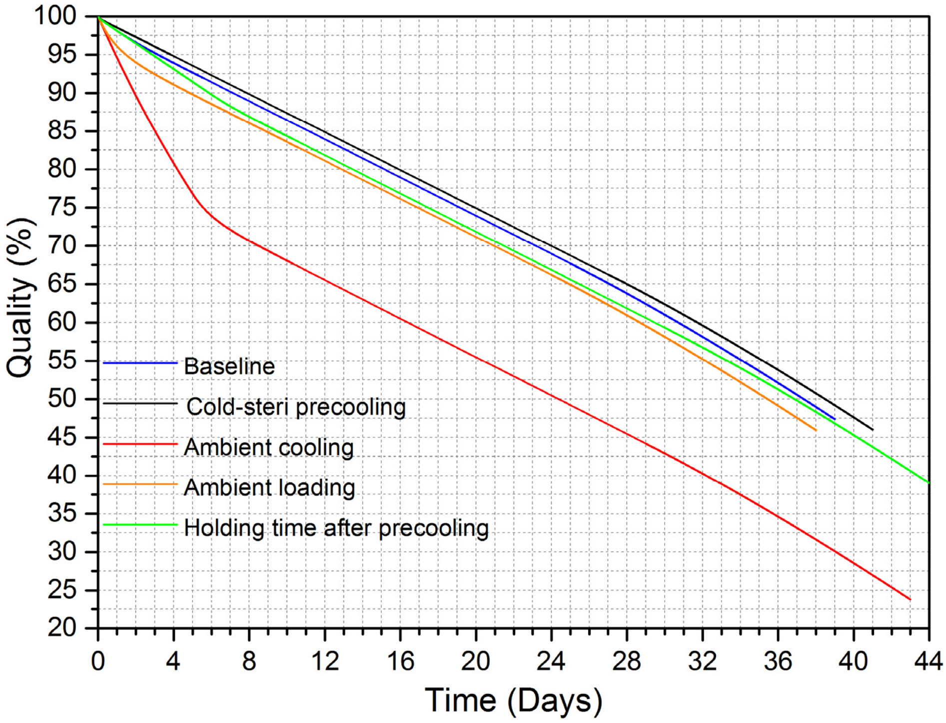

Fig. 10 Average Quality loss of all fruit in the five cold chains.

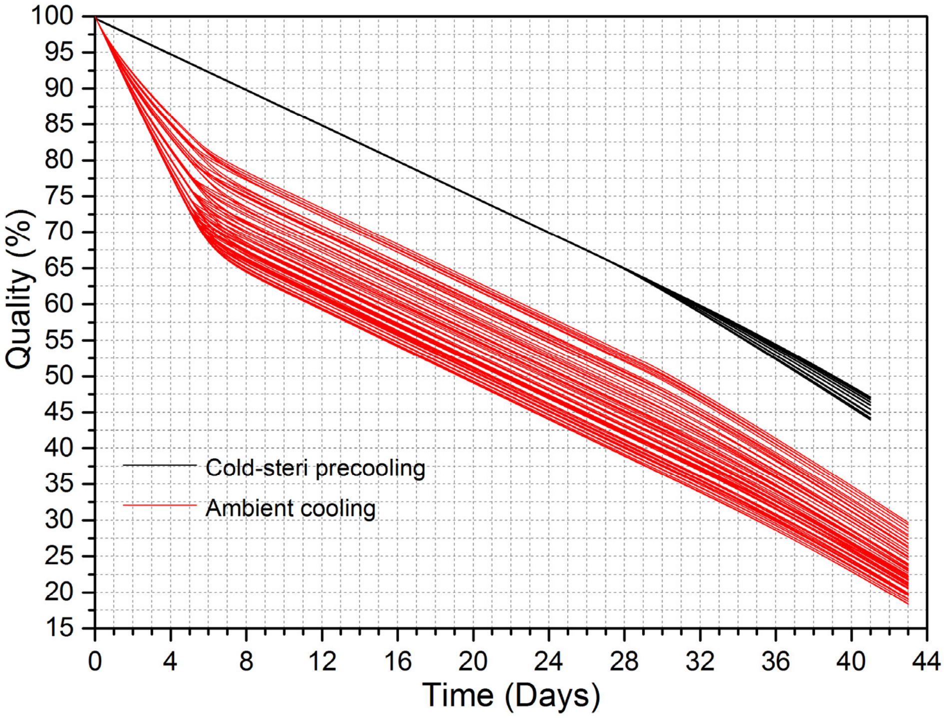

Fig. 11 Quality loss of individual fruit in the first and second alternative cold chain.

Table 1 Different cold chains.

Cold chain	Precooling			Cold storage before shipment			Refrigerated transport			Cold storage after shipment		
	Air flow rate (L $kg^{-1}s^{-1}$)	Set point temperature (°C)	Duration (days)	Air flow rate (L $kg^{-1}s^{-1}$)	Set point temperature (°C)	Duration (days)	Air flow rate (L $kg^{-1}s^{-1}$)	Set point temperature (°C)	Duration (days)	Air flow rate (L $kg^{-1}s^{-1}$)	Set point temperature (°C)	Duration (days)
Baseline	1	3	1	-	-	-	0.02	-1	24	0.002	4	14
Cold-steri precooling	1	-1	3	-	-	-	0.02	-1	24	0.002	4	14
Ambient cooling	-	-	-	0.002	3	5	0.02	-1	24	0.002	4	14
Ambient loading	-	-	-	-	-	-	0.02	-1	24	0.002	4	14
Holding time after precooling	1	3	1	0.002	3	5	0.02	-1	24	0.002	4	14

- The cold chain does not contain the corresponding unit operation.